Simultaneous dimension reduction and multi-objective clustering

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Dimension reduction and clustering

Summarize the data

- **Dimension reduction:** find some principal components explaining the major *variability* in the data
- **Clustering:** find some clusters explaining the major *heterogeneity* of the data

Link between dimension reduction and clustering

Often when visualizing the data, one is interested in *visualizing clusters* on the *visualization space*.

In practice

Dimension reduction and clustering are performed separately or sequentially but rarely simultaneously.

Combining dimension reduction and clustering through probabilistic models

Generative models allow to combine visualization and clustering

- Tibshirani & Hastie (1996): Reduced rank discriminant analysis
- Kumar & Andreou (1998): Heteroscedastic discriminant analysis
- Bouveyron & Brunet (2012): Model-based clustering and visualization in the Fisher discriminative subspace

In a rigorous probabilistic way

- A unique homogeneous criterion to optimize: the likelihood
- Simultaneous selection of the number clusters and of the number of components: BIC
- Missing data naturally taken into account: EM algorithm

Multi-objective clustering

Motivation: clustering part

- Usually clustering summarizes the data information by only **one** latent variable, the cluster variable.
- But we would like to allow for several views of the data with potentially **several cluster variable**.
- Often performances of clustering methods measured based on classification of reference, but many possible references in many settings (sex, species, status, ...).

Motivation: visualisation part

- View each clustering variable on a **clustering component**
- Heterogeneity-based visualisation rather than inertia-based visualisation

Illustration (1/2)

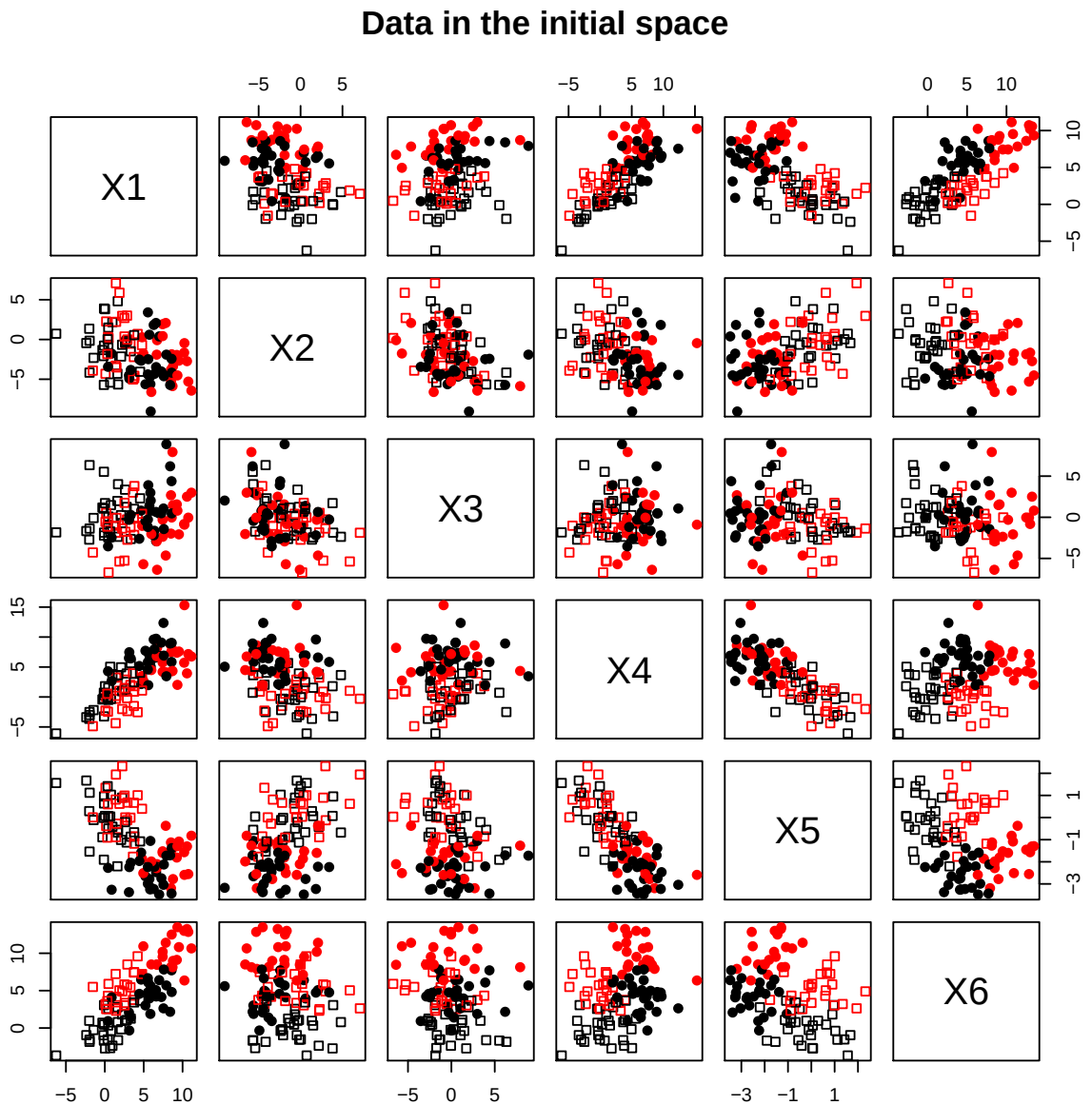
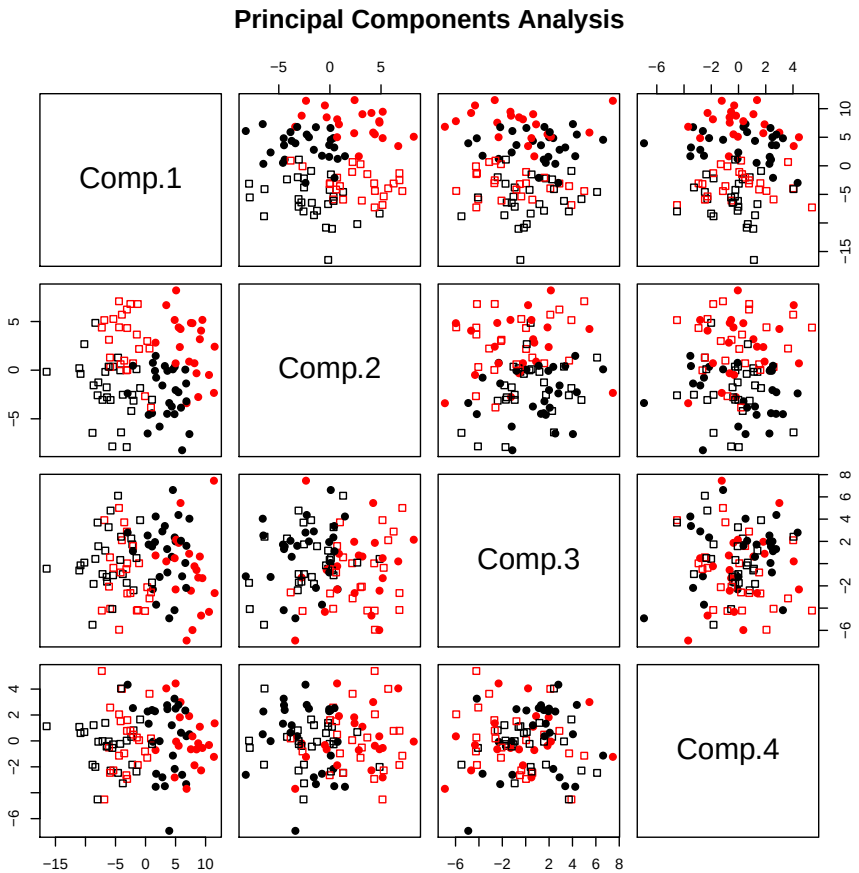
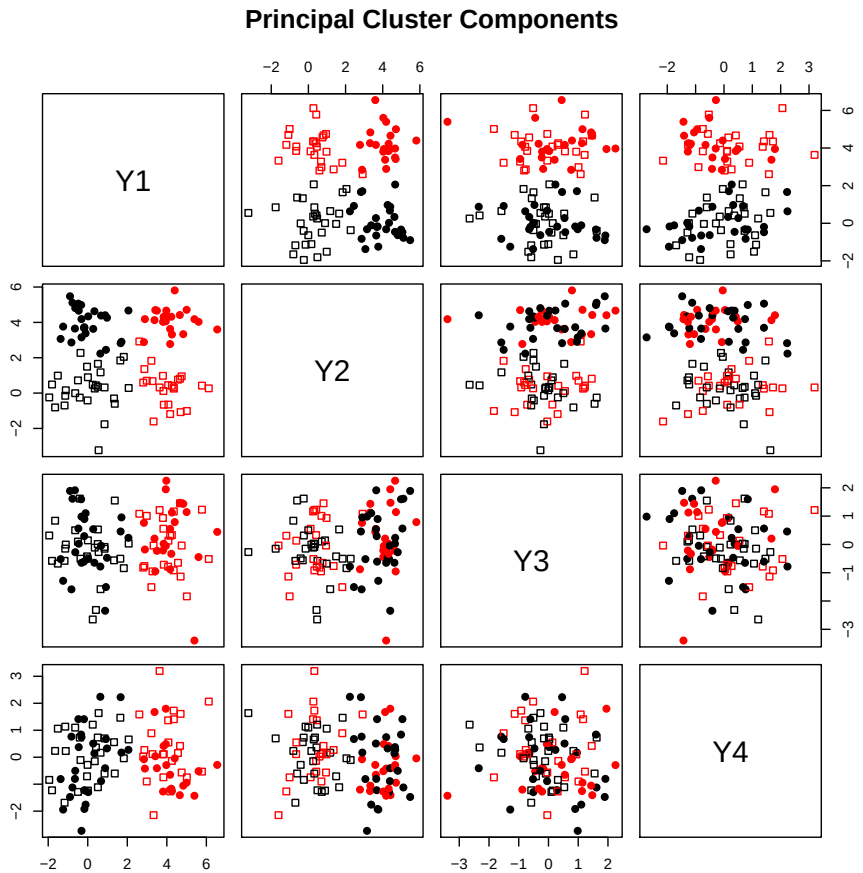


Illustration (2/2)





Outline

1. Multi-objective mixture model

2. Parameters estimation

3. Experiments on simulated and real datasets

Presentation of the model

Generative process

- Draw H independent class variables
  - $\boldsymbol{z}^1, \ldots, \boldsymbol{z}^H$ with $K_1, \ldots, K_H$ modalities
  - $p(z_k^h = 1) = \pi_k^h$
- Draw H classifying latent variables
  - $\boldsymbol{y}^h \in \mathbb{R}^{p_h}$ with $p_h \leq K_h - 1$
  - $\boldsymbol{y}^h | z_k^h = 1 \sim \mathcal{N}_{p_h}(\boldsymbol{\nu}_k^h, I_{p_h})$
- Draw non classifying latent variables
  - $\boldsymbol{u} \in \mathbb{R}^{d-p_\bullet}$ with $p_\bullet = \sum_{h=1}^{H} p_h$
  - $\boldsymbol{u} \sim \mathcal{N}_{d-p_\bullet}(\gamma, I_{d-p_\bullet})$
- Compute $\boldsymbol{x}$ ($\boldsymbol{x} \in \mathbb{R}^d$) defined by:

$$\boldsymbol{x} = \boldsymbol{A} \begin{pmatrix} \boldsymbol{y}^1 \\ \vdots \\ \boldsymbol{y}^H \\ \boldsymbol{u} \end{pmatrix}, \text{ where } \boldsymbol{A} \in \mathcal{M}_{d,d}(\mathbb{R})$$

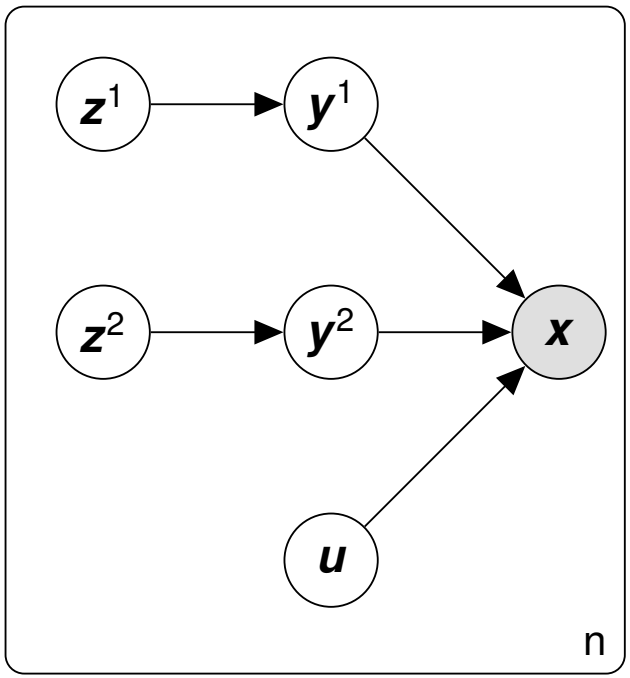


Illustration for $H = 2$

Properties of the model

- The classifying variables $\boldsymbol{y}^1, \ldots, \boldsymbol{y}^H$ are
  - independant
  - follow a mixture

  $\Rightarrow$ allow to visualize the data on different clustering projections
- The probability distribution function of $\boldsymbol{x}$ can simply be written

$$p(\boldsymbol{x}) = \frac{1}{|\boldsymbol{A}|} p(\boldsymbol{u}) \prod_{h=1}^{H} p(\boldsymbol{y}^h)$$

- For sake of simplicity we will rather work with the inverse of $\boldsymbol{A}$ defined by $\boldsymbol{A}^{-1} = \begin{pmatrix} \boldsymbol{V}_1 \\ \vdots \\ \boldsymbol{V}_H \\ \boldsymbol{R} \end{pmatrix}$, such that $\boldsymbol{y}^h = \boldsymbol{V}_h \boldsymbol{x}$

Estimation strategy

Goal

Estimate $\boldsymbol{V}_1,\ldots,\boldsymbol{V}_H$, $\boldsymbol{R}$ and the mixture parameters of the distributions of $\boldsymbol{y}^1,\ldots,\boldsymbol{y}^H$

Maximum likelihood estimation through a GEM algorithm

- E-step easy to perform
- M-step hard to perform with respect to $\boldsymbol{V}_1,\ldots,\boldsymbol{V}_H$, $\boldsymbol{R}$
  - perform alternate optimization on clustering projections
  - each optimization relying on a reduced rank linear discriminant analysis

Detail of the GEM algorithm

EM algorithm

Until convergence, for $h \in \{1, \ldots, H\}$ iterate the following steps:

- E step: compute

$$t_{ik}^{h\,(r+1)} = p(\boldsymbol{z}_i^h | \boldsymbol{x}_i; \boldsymbol{\theta}^{(r)}) = \frac{\pi_k \phi_{p_h}(\boldsymbol{V}_h^{(r)} \boldsymbol{x}; \boldsymbol{\nu}_k^{h\,(r)}, \boldsymbol{I}_{p_h})}{\sum_{k'=1}^{K} \pi_{k'} \phi_{p_h}(\boldsymbol{V}_h^{(r)} \boldsymbol{x}; \boldsymbol{\nu}_{k'}^{h\,(r)}, \boldsymbol{I}_{p_h})}$$

- M step: update $\boldsymbol{V}_h$, $\boldsymbol{R}$, $\boldsymbol{\nu}_1^h, \ldots, \boldsymbol{\nu}_{K_h}^h$, $\pi_1^h, \ldots, \pi_{K_h}^h$ and γ

Detail of the M step

- Constrain $\boldsymbol{V}_h^{(r+1)}$ and $\boldsymbol{R}^{(r+1)}$ to be linear combinations of $\boldsymbol{V}_h^{(r)}$ and $\boldsymbol{R}^{(r)}$, the parameters of other clustering dimension being fixed:

$$\begin{pmatrix} \boldsymbol{V}_h^{(r+1)} \\ \boldsymbol{R}^{(r+1)} \end{pmatrix} = \boldsymbol{M} \begin{pmatrix} \boldsymbol{V}_h^{(r)} \\ \boldsymbol{R}^{(r)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{M}_1 \\ \boldsymbol{M}_2 \end{pmatrix} \begin{pmatrix} \boldsymbol{V}_h^{(r)} \\ \boldsymbol{R}^{(r)} \end{pmatrix},$$

- by denoting $\boldsymbol{y}^{h(r)} = \boldsymbol{V}_h^{(r)} \boldsymbol{x}$ and $\boldsymbol{u}^{(r)} = \boldsymbol{R}^{(r)} \boldsymbol{x}$,
- finding $\boldsymbol{M}$ and other parameters is equivalent to perform reduced rank linear discriminant analysis on the data $\begin{pmatrix} \boldsymbol{y}^{h(r)} \\ \boldsymbol{u}^{(r)} \end{pmatrix}$ weighted by $t_{ik}^{h\,(r+1)}$

Possible models and number of parameters

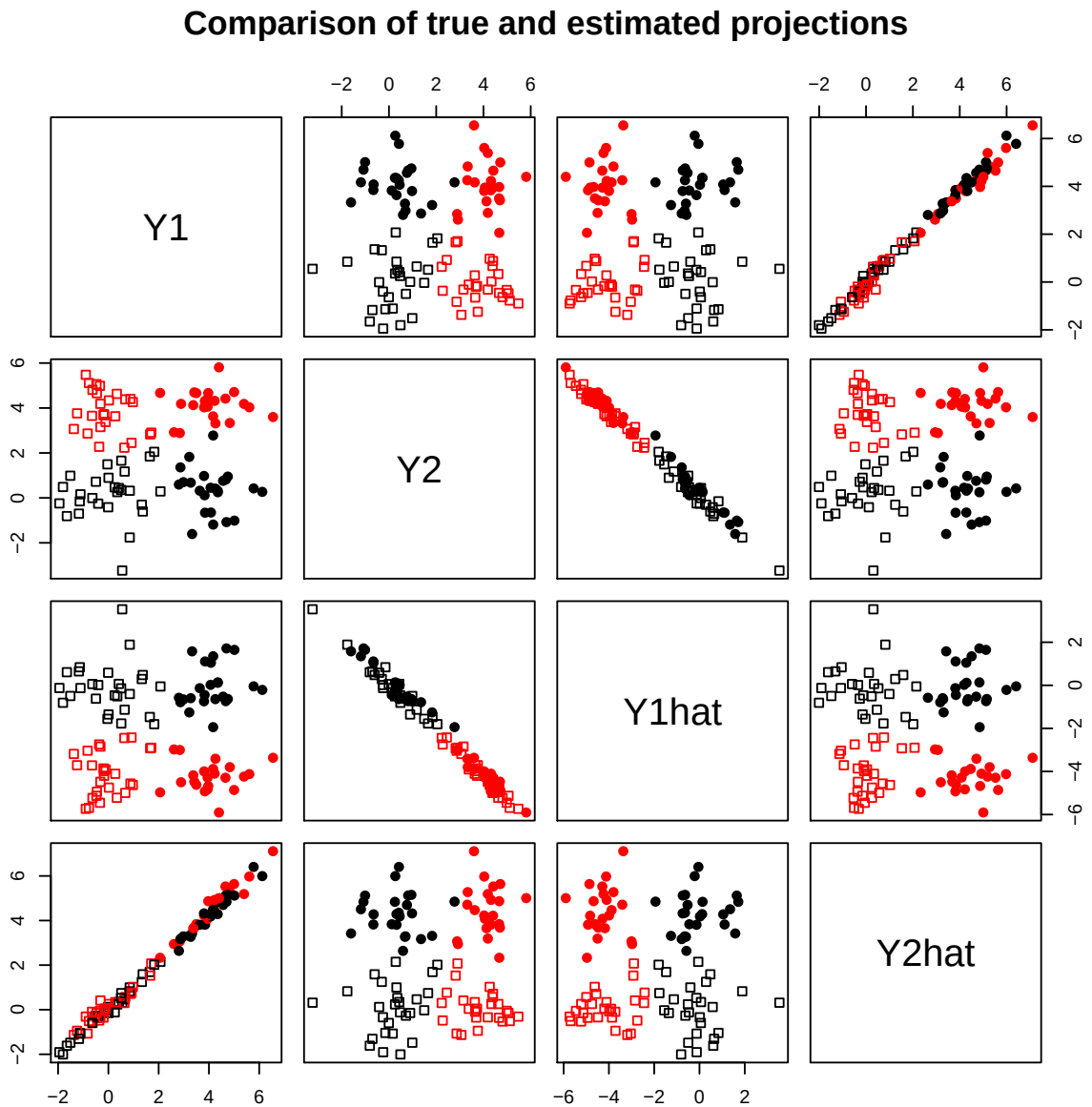
Remarks

- Need to choose H, $K_1, \ldots, K_H$ and $p_1, \ldots, p_H$: possible selection by model choice.
- $\boldsymbol{V}_1, \ldots, \boldsymbol{V}_H$ and $\boldsymbol{R}$ estimated up to isometric transformations.

Number of parameters

$$\dim(\Theta) = \sum_{h=1}^{H}(K_h - 1) + \sum_{h=1}^{H} \frac{p_h(2K_h + 2d - p_h + 1)}{2} + \frac{(d - p_\bullet)(d + p_\bullet + 3)}{2}$$

Simulated data set: illustration



Simulated data: model choice

- Performed using the BIC criterion

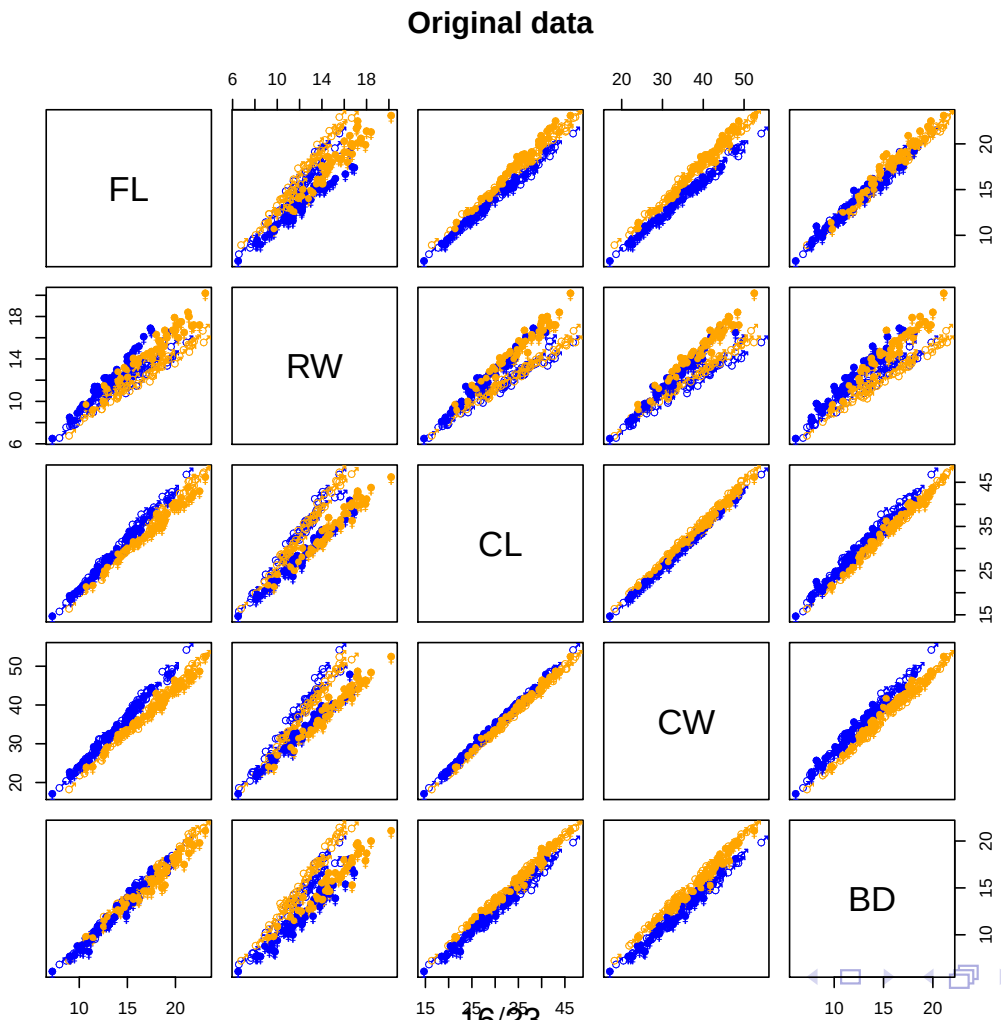
$$BIC = \ell(\boldsymbol{x}; \hat{\boldsymbol{\theta}}) - \frac{\dim(\Theta)}{2} \log n$$

- Model collection: $H = 2$, $K_1 \in \{1, \ldots, 5\}$, $K_2 \in \{1, \ldots, 5\}$, $p_1 = p_2 = 1$

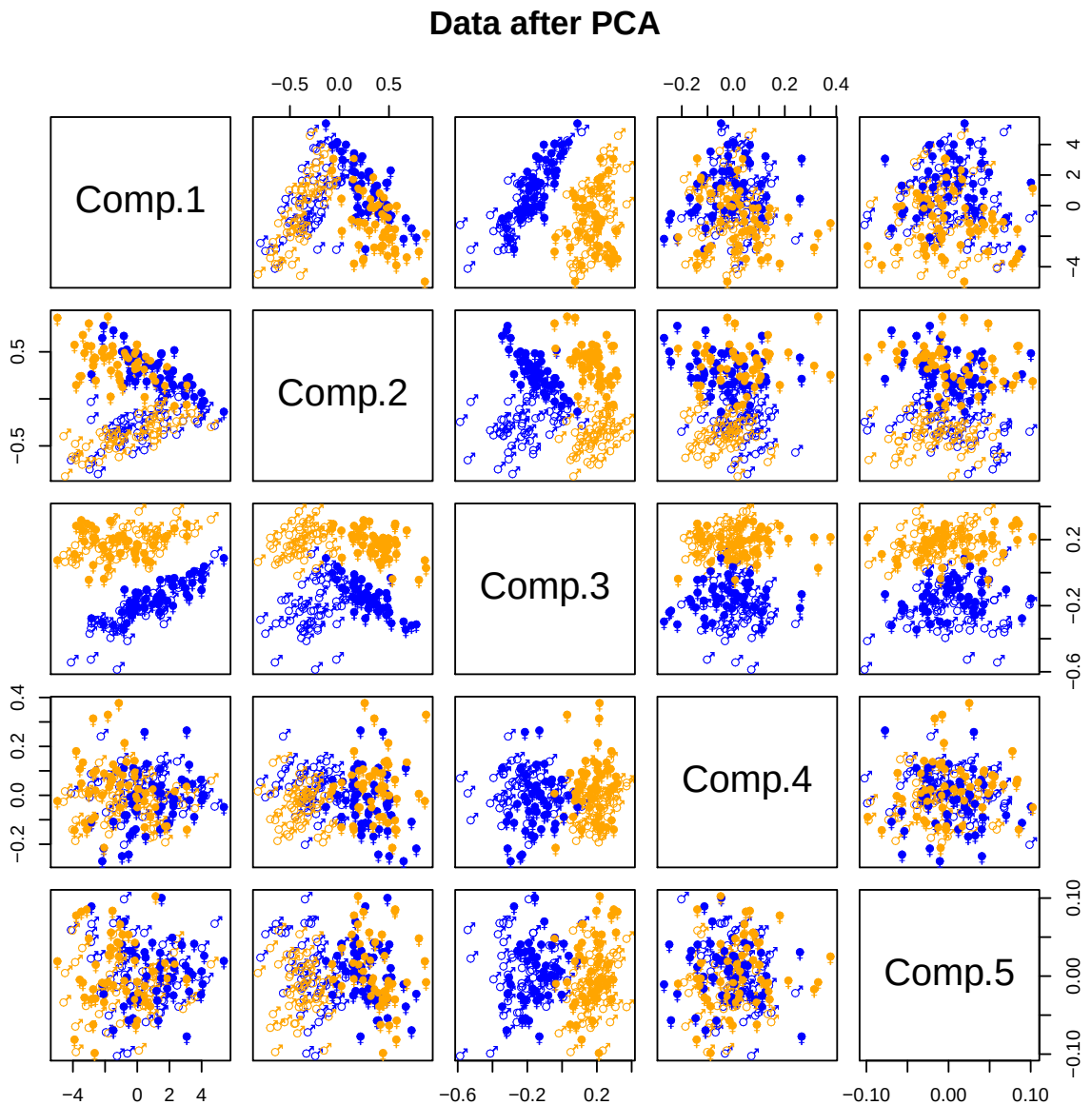
$K_1 \setminus K_2$	1	2	3	4	5
1	-1414.69	-1395.53	-1397.55	-1395.65	-1396.88
2		**-1383.76**	-1384.64	-1397.17	-1393.86
3			-1384.05	-1396.36	-1395.36
4				-1392.30	-1394.01
5					-1389.14

Crabs data set

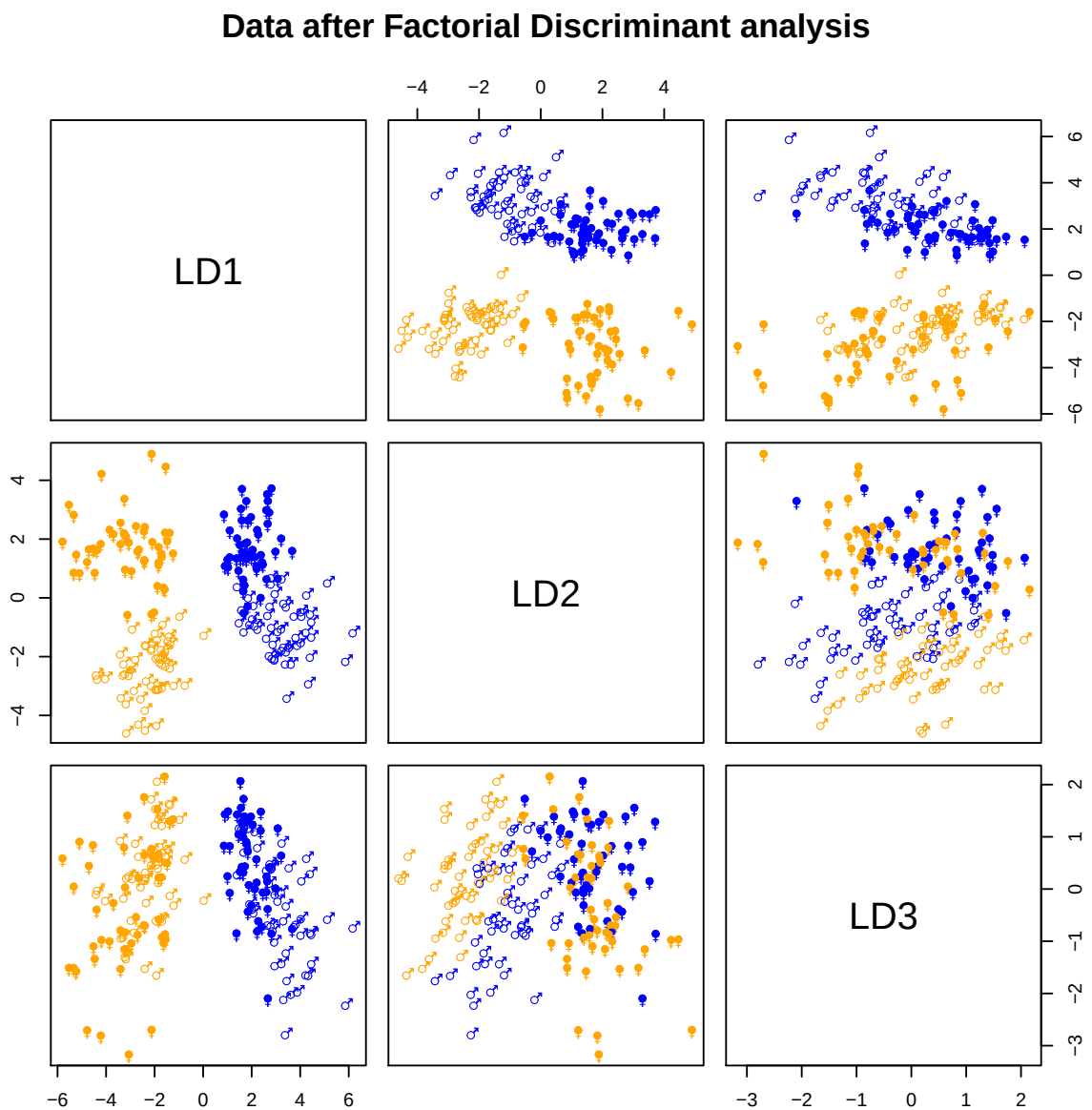
200 crabs morphological data, 5 morphological variables, 50 males orange, 50 males blue, 50 females orange, 50 females blue.



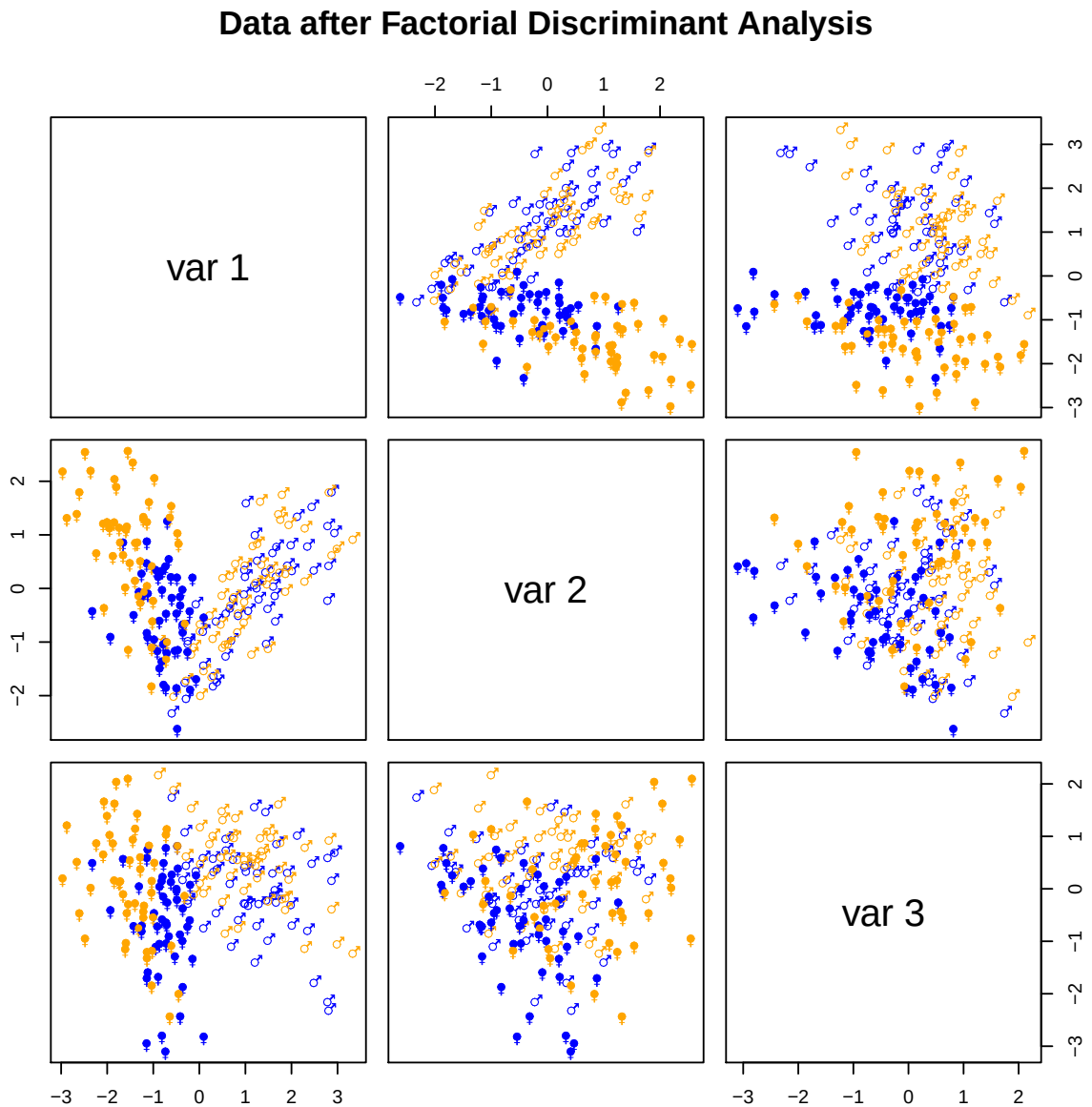
PCA on the crab data set



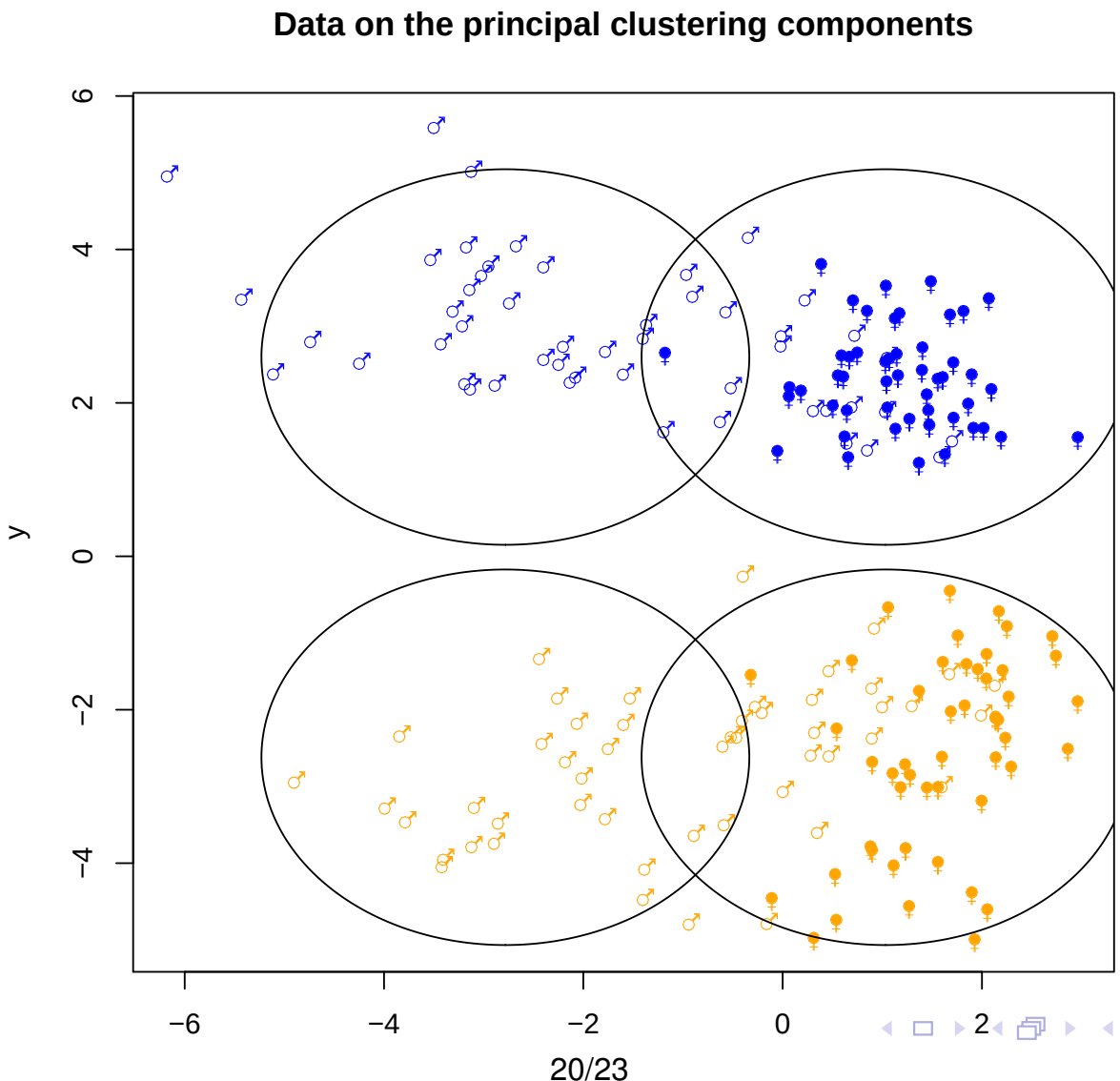
FDA on the crab data set: supervised setting



FDA on the crab data set: unsupervised setting



Principal clustering components: $H = 2$, $K_1 = K_2 = 2$, $p_1 = p_2 = 1$

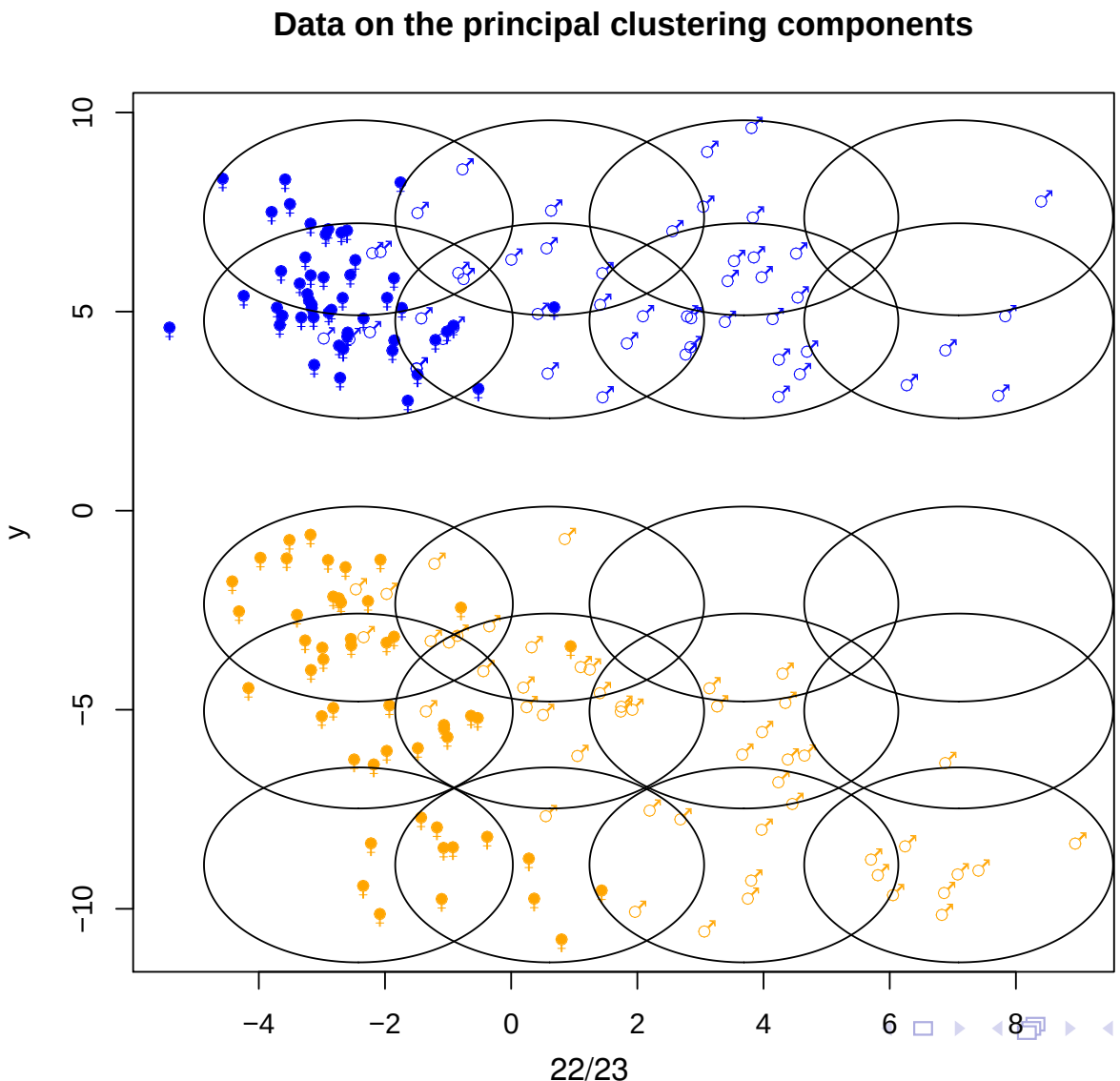


Principal clustering components: model choice

- Performed using the BIC criterion
- Model collection: $H = 2$, $K_1 \in \{1, \ldots, 5\}$, $K_2 \in \{1, \ldots, 5\}$, $p_1 = p_2 = 1$

$K_1 \setminus K_2$	1	2	3	4	5
1	-313.02	-252.35	-244.20	-250.60	-249.40
2		**-229.73**	-254.76	-254.82	-233.91
3			-248.82	-255.49	-233.17
4				-238.88	-231.19
5					-269.75

Principal clustering components: $H = 2$, $K_1 = 4$, $K_2 = 5$, $p_1 = p_2 = 1$



Conclusion and perspectives

Conclusion

- model combining visualization and clustering with many clustering view points
- possibility to perform model choice

Perspectives

- consider sparse estimates of the $\boldsymbol{A}$ matrix for the high dimensional setting
- extension to the heteroscedastic setting
- extension for model based variable clustering

Linear discriminant analysis (LDA)

Data

- $\boldsymbol{x} \in \mathbb{R}^d$: the observed continuous variables
- $\boldsymbol{z} \in \{1, \ldots, K\}$: the cluster (latter considered as unknown)

Assumptions

n independent replicates of $(\boldsymbol{x}, \boldsymbol{z})$

- $\boldsymbol{z} \sim Mult(\pi_1, \ldots, \pi_K)$ with $\pi_k = p(z_k = 1)$
- $\forall k \in \{1, \ldots, K\}, \quad \boldsymbol{x} | z_k = 1 \sim \mathcal{N}_d(\boldsymbol{\mu}_k, \boldsymbol{\Sigma})$

Parameters estimation

$\hat{\pi}_k = \frac{n_k}{n}$, $\hat{\boldsymbol{\mu}}_k = \bar{\boldsymbol{x}}_k$ and $\hat{\boldsymbol{\Sigma}} = \boldsymbol{W}$ (empirical within-class covariance matrix)

Classification

$$p(z_k = 1 | \boldsymbol{x}, \hat{\boldsymbol{\theta}}) = \frac{\hat{\pi}_k \phi_d(\boldsymbol{x}; \hat{\boldsymbol{\mu}}_k, \hat{\boldsymbol{\Sigma}})}{\sum_{k'=1}^{K} \hat{\pi}_{k'} \phi_d(\boldsymbol{x}; \hat{\boldsymbol{\mu}}_{k'}, \hat{\boldsymbol{\Sigma}})} \Rightarrow \hat{\boldsymbol{z}} = \underset{k \in \{1, \ldots, K\}}{\text{argmax}} \; \hat{\boldsymbol{\mu}}_k^\top \hat{\boldsymbol{\Sigma}}^{-1} \boldsymbol{x} - \frac{1}{2} \boldsymbol{\mu}_k^\top \hat{\boldsymbol{\Sigma}}^{-1} \boldsymbol{\mu}_k - \log(\hat{\pi}_k)$$

$\Rightarrow$ linear classification boundary.

Factorial discriminant analysis (FDA)

FDA principle

- The first component of FDA finds $\boldsymbol{v}_1 \in \mathbb{R}^d$ maximizing the variance explained by the cluster:

$$\boldsymbol{v}_1 = \arg\max_{\boldsymbol{v}\in\mathbb{R}^d} \frac{\boldsymbol{v}^\top \boldsymbol{B}\boldsymbol{v}}{\boldsymbol{v}^\top(\boldsymbol{W}+\boldsymbol{B})\boldsymbol{v}} = \arg\max_{\boldsymbol{v}\in\mathbb{R}^d} \frac{\boldsymbol{v}^\top \boldsymbol{B}\boldsymbol{v}}{\boldsymbol{v}^\top \boldsymbol{W}\boldsymbol{v}}$$

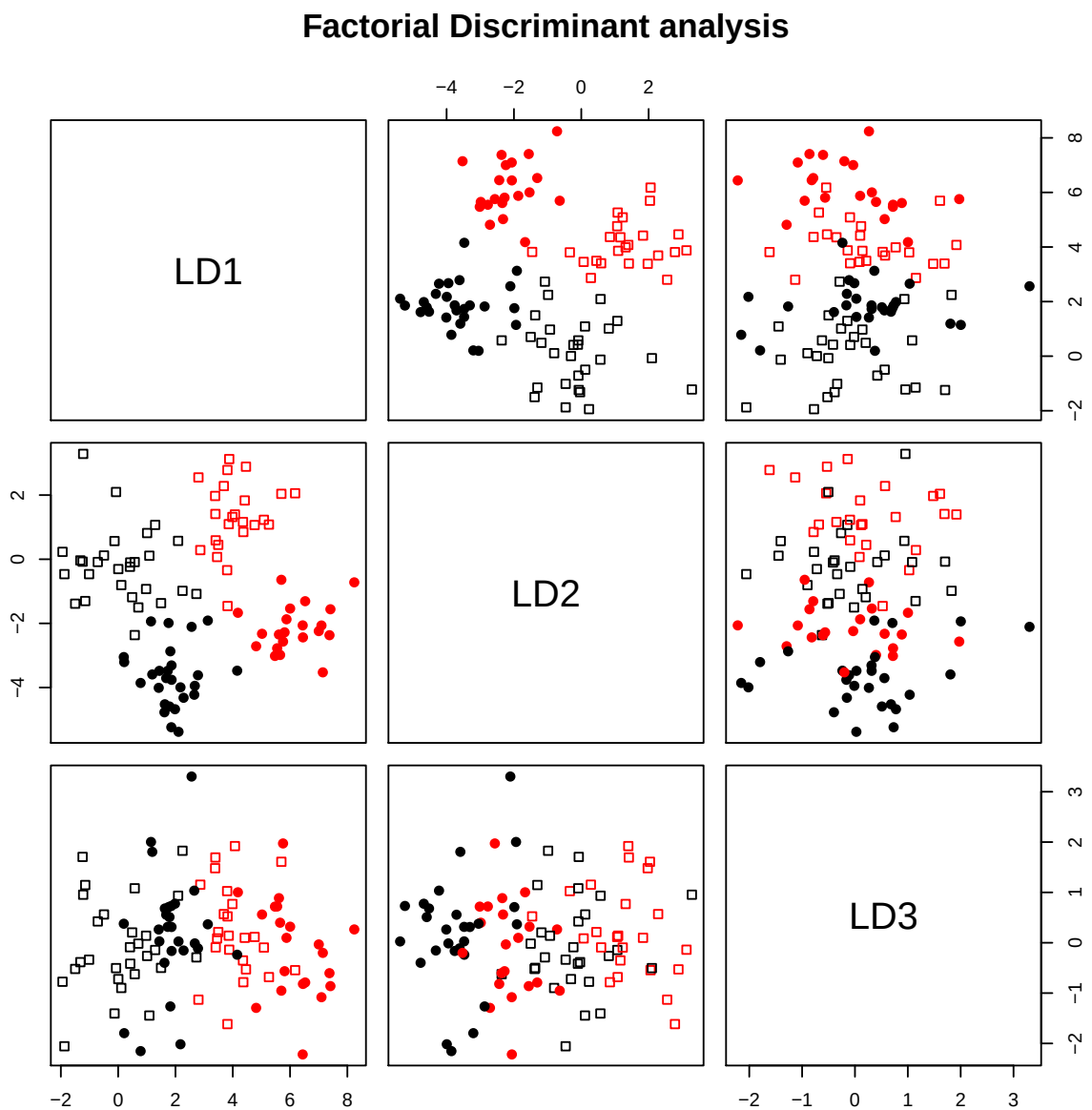
  with $\boldsymbol{B}$ the empirical between class covariance matrix.
- $\boldsymbol{v}_1$ is given by the eigen vector associated with the highest eigen value of $\boldsymbol{W}^{-1}\boldsymbol{B}$
- The remaining discriminant components are obtained through the remaining eigen vectors of $\boldsymbol{W}^{-1}\boldsymbol{B}$

Remark: The number of non null eigen-values of $\boldsymbol{W}^{-1}\boldsymbol{B}$ is at most $\min(d, K-1)$.

Classification rule

If components within class variance is scaled to one, classification can be performed by nearest class center with the Euclidean distance on the projected data.

Illustration of FDA



Equivalence between LDA and FDA

Campbell (1984)

FDA $\Leftrightarrow$ LDA s.c. rank$(\{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K\}) = p$, where $p \leq K - 1$.

Reparametrization of LDA under constrains

$$\boldsymbol{x}|z_k = 1 \sim \mathcal{N}_d\left(\boldsymbol{A}\begin{pmatrix}\boldsymbol{\nu}_k \\ \boldsymbol{\gamma}\end{pmatrix}, \boldsymbol{A}\boldsymbol{A}^\mathsf{T}\right)$$

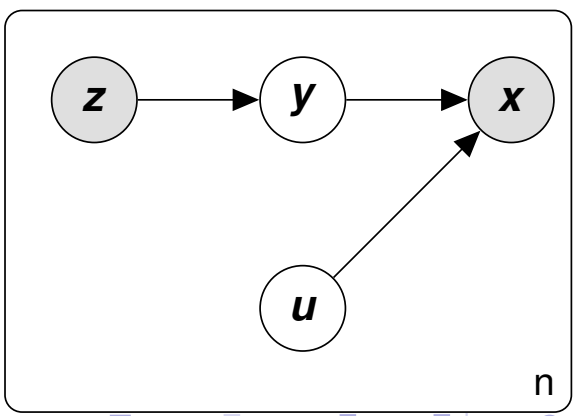
where $\boldsymbol{\nu}_k \in \mathbb{R}^p$, $\boldsymbol{\gamma} \in \mathbb{R}^{d-p}$ and $\boldsymbol{A} \in \mathcal{M}_{d,d}(\mathbb{R})$.

Generative interpretation

Let $\boldsymbol{y} \in \mathbb{R}^p$ and $\boldsymbol{u} \in \mathbb{R}^{d-p}$. The generative model is:

- Draw $\boldsymbol{z}$: $\boldsymbol{z} \sim \mathit{Mult}(1; \pi_1, \ldots, \pi_K)$
- Draw $\boldsymbol{y}|\boldsymbol{z}$: $\boldsymbol{y}|z_k = 1 \sim \mathcal{N}_p(\boldsymbol{\nu}_k, \boldsymbol{I}_p)$
- Draw $\boldsymbol{u}$: $\boldsymbol{u} \sim \mathcal{N}_{d-p}(\boldsymbol{\gamma}, \boldsymbol{I}_{d-p})$
- Compute $\boldsymbol{x}$ based on $\boldsymbol{y}$ and $\boldsymbol{u}$:

$$\boldsymbol{x} = \boldsymbol{A}\begin{pmatrix}\boldsymbol{y} \\ \boldsymbol{u}\end{pmatrix}$$



Posterior class membership probabilities

Posterior probabilities

Let $\boldsymbol{V} \in \mathcal{M}_{p,d}(\mathbb{R})$ and $\boldsymbol{R} \in \mathcal{M}_{d-p,d}(\mathbb{R})$ the matrices such that $\boldsymbol{y} = \boldsymbol{V}\boldsymbol{x}$, $\boldsymbol{u} = \boldsymbol{R}\boldsymbol{x}$. Obviously $\begin{pmatrix} \boldsymbol{V} \\ \boldsymbol{R} \end{pmatrix} = \boldsymbol{A}^{-1}$.

$$p(z_k = 1|\boldsymbol{x}) = p(z_k = 1|\boldsymbol{y}, \boldsymbol{u}) = p(z_k = 1|\boldsymbol{y}) = p(z_k = 1|\boldsymbol{V}\boldsymbol{x}).$$

$\boldsymbol{V}\boldsymbol{x}$ conveys all the clustering information.

$$p(z_k = 1|\boldsymbol{x}) = \frac{\pi_k \phi_p(\boldsymbol{V}\boldsymbol{x}; \boldsymbol{\nu}_k, \boldsymbol{I}_p)}{\sum_{k'=1}^{K} \pi_{k'} \phi_p(\boldsymbol{V}\boldsymbol{x}; \boldsymbol{\nu}_{k'}, \boldsymbol{I}_p)}.$$

Parameters estimation

$$\ell(\boldsymbol{\theta}; \mathbf{x}, \mathbf{z}) = n \log \left| \det \begin{pmatrix} \boldsymbol{V} \\ \boldsymbol{R} \end{pmatrix} \right| - \overbrace{\frac{1}{2} \sum_{i=1}^{n} \sum_{k=1}^{K} z_{ik} \| \boldsymbol{V}\boldsymbol{x}_i - \boldsymbol{\nu}_k \|^2}^{\textbf{classifiying}}$$
$$\underbrace{-\frac{1}{2} \sum_{i=1}^{n} \| \boldsymbol{R}\boldsymbol{x}_i - \gamma \|^2}_{\textbf{not classifying}} - \frac{n}{2} \log(2\pi) + \sum_{i=1}^{n} \sum_{k=1}^{K} z_{ik} \log(\pi_k).$$

Maximum likelihood estimation

- $\hat{\boldsymbol{V}}$ and $\hat{\boldsymbol{R}}$ are obtained through eigen value decomposition of $\boldsymbol{W}^{-1}\boldsymbol{B}$.
- $\hat{\nu}_1, \ldots, \hat{\nu}_K$ and $\hat{\gamma}$ explicit given $\hat{\boldsymbol{V}}$ and $\hat{\boldsymbol{R}}$.